

ON THE MAXIMAL EXCESS CHARGE OF THE CHANDRASEKHAR-COULOMB HAMILTONIAN IN TWO DIMENSIONS

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ABSTRACT. We show that for the straightforward quantized relativistic Coulomb Hamiltonian of a two-dimensional atom – or the corresponding magnetic quantum dot – the maximal number of electrons does not exceed twice the nuclear charge. The result is then generalized to the presence of external magnetic fields and atomic Hamiltonians. This is based on the positivity of

$$|\mathbf{x}|T(\mathbf{p}) + T(\mathbf{p})|\mathbf{x}|$$

which – in two dimensions – is false for the non-relativistic case $T(\mathbf{p}) = \mathbf{p}^2/2$, but is proven in this paper for $T(\mathbf{p}) = |\mathbf{p}|$, i.e., the ultra-relativistic kinetic energy.

1. INTRODUCTION

The energy of two-dimensional quantum systems interacting via three dimensional Coulomb-like potentials like graphene in a background magnetic field given by a vector potential \mathfrak{A} is given by the quadratic form

$$(1) \quad \mathcal{E}[\psi] = (\psi, W_n \psi)$$

where ψ is a sufficiently smooth element from the Hilbert space $\mathfrak{H}_{\mathfrak{A}}$ built from states above the Fermi level:

$$(2) \quad \psi \in \mathfrak{H}_{\mathfrak{A}} := \Lambda^+[L^2(\mathbb{R}^2 : \mathbb{C}^2)] , \quad \Lambda^+ := \chi_{(0,\infty)}(D_{\mathfrak{A}}).$$

(Note that this model is physically relevant for large gaps and relatively small interactions. For strong interactions and small gaps a field theoretic description allowing for particle-hole creation and annihilation is required (Paananen and Egger [10]).) The operator

$$(3) \quad W_N := \sum_{n=1}^N (T_{\mathfrak{A},n} + e\boldsymbol{\sigma}_n \cdot \mathbf{A}(\mathbf{x}_n) - e\varphi(\mathbf{x}_n)) + \sum_{1 \leq m < n \leq N} \frac{e^2}{|\mathbf{x}_m - \mathbf{x}_n|}$$

is the multi-particle Weyl operator (massless Dirac operator) with kinetic energy $T_{\mathfrak{A}} := \boldsymbol{\sigma} \cdot (\mathbf{p} + e\mathfrak{A})$ where $-e$ is the charge of the electron. The Hamiltonian is defined via the quadratic form. The Hamiltonian

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has been used to describe multi-particle effects of graphene quantum dots (see Egger et al [1] where its basic mathematical properties have been discussed). The electro-magnetic potentials φ and \mathfrak{A} are defining the quantum dot.

To be concrete we mention that the choice used by Egger et al [1] (see also Paananen et al [11]) would be allowed, namely to take $\mathfrak{A} = \mathfrak{A}_0 + \mathbf{A}_0$ and $\mathbf{A} = 0$ with

$$(4) \quad \mathfrak{A}_0(\mathbf{x}) = \frac{B}{2} \begin{pmatrix} -x_2 \\ x_1 \end{pmatrix},$$

i.e., we have a homogeneous magnetic field of strength B orthogonal to the x_1 - x_2 -plane, and

$$(5) \quad \mathbf{A}_0(\mathbf{x}) := -\frac{BR^2}{2|\mathbf{x}|^2} \begin{pmatrix} -x_2 \\ x_1 \end{pmatrix} \begin{cases} \frac{|\mathbf{x}|^2}{R^2} & |\mathbf{x}| \leq R \\ 1 & |\mathbf{x}| > R, \end{cases}$$

the potential that eliminates the magnetic field in a circle of radius R but leaves the field unchanged outside. In total this is a homogeneous magnetic field with a cavity of radius R around the origin. As electric field we could choose $\varphi(\mathbf{x}) = eZ/|\mathbf{x}|$, i.e., the potential of a defect atom placed at the origin.

An alternative approach would be to take $\mathfrak{A} = \mathfrak{A}_0$, i.e., define the vacuum with respect to the homogeneous magnetic field, and to pick $\mathbf{A} = \mathbf{A}_0$. Although for weak fields these two will yield similar results they are not identical. Nevertheless, by the variational principle for eigenvalues in gaps [3], the latter will bound the former from below. In addition it allows for a more direct treatment of the excess charge problem. Because of this, we will direct our attention on the second choice.

The corresponding quadratic form on $\bigwedge_{n=1}^N \Lambda^+[C_0^\infty(\mathbb{R}^2 : \mathbb{C}^2)]$ is bounded from below, if and only if

$$Z \leq \left(\frac{\Gamma(\frac{1}{4})^4}{8\pi^2} + \frac{8\pi^2}{\Gamma(\frac{1}{4})} \right)^{-1}$$

independently of the strength of the field \mathfrak{A} [7]. Egger et al [1] studied also numerically how many electrons a quantum dot is able to bind in the context of a mean-field model. However the question of bounding the total number of electrons localized in the quantum dot was left unanswered. In the sequel we will address this question, however not for the no-pair Hamiltonian defined by the quadratic form of W_N in $\bigwedge_{n=1}^N \mathfrak{H}_{\mathfrak{A}}$ but for the corresponding Chandrasekhar type operator $C_{\mathbf{A}, \varphi, N}$, i.e., W_N with $T_{\mathfrak{A}}$ replaced by $|T_{\mathfrak{A}}|$ self-adjointly realized in $L^2(\mathbb{R}^{3N} : \mathbb{C}^{2N})$ with domain $H^1(\mathbb{R}^{3N} : \mathbb{C}^{2N})$. Again by the variational principle, the eigenvalues of this operator bound the eigenvalues of the no-pair operator from below, since the quadratic form of the no-pair operator is just a restriction of the Chandrasekhar case.

An a priori bound on the maximal number of electrons that can be bound has been derived by Lieb [5] for relativistic and non-relativistic Coulomb Hamiltonians in three dimensions. The idea of the proof is to multiply the Schrödinger equation by $|\mathbf{x}_1|\psi(x)$ and to integrate. It yields – in the atomic case – the bound $N < 2Z + 1$ and rests on the inequality

$$(6) \quad 0 \leq |\mathbf{x}|T + T|\mathbf{x}|.$$

For the non-relativistic kinetic $T = \mathbf{p}^2/2$ (8) is equivalent to a Hardy inequality which is true in three dimensions but false in two dimension. The case of the relativistic kinetic energy $T = |\mathbf{p}|$ is reduced by Lieb [5] to the non-relativistic case. In other words, it is not clear a priori whether (8) holds. The purpose of this paper is to show this inequality and apply it to the Hamiltonian $C_{\mathbf{A},\varphi,N}$ of the quantum dot.

Before we actually do this we remark:

- In three dimensions Nam[8] improved Lieb's result for the non-relativistic Schrödinger operator and $Z \geq 6$. He could show the bounds $N < 1.22Z + 3Z^{\frac{1}{3}}$ using similar ideas.
- In two dimension, the above failure of positivity of (8) can be controlled using an idea of Seiringer [12] and Nam and Solovej [9]: Since the eigenvalues of the two-dimensional hydrogen atoms (two-dimensional Kepler problem) are $-Z^2/2(n+1/2)^2$ (Flügge and Marschall [2, Problem 24] each of multiplicity $2n+1$ ($e = 1$)). This gives $(\psi, |\mathbf{x}_1|^{-1}\psi) \leq 4 \log(Z^{1/2}) + 10$ for the ground state of the N particle system which in turn yields

$$(7) \quad N \leq 2Z + \log(Z^{1/2}) + \frac{7}{2}.$$

2. MAIN INEQUALITY

Our basic result is

Theorem 1. *Assume $\mathfrak{A} \in L^2_{\text{loc}}(\mathbb{R}^2 : \mathbb{C}^2)$, $\mathbf{p} := -i\nabla$, and $T_{\mathfrak{A}} := |\mathbf{p} + \mathfrak{A}|$, then*

$$(8) \quad |\mathbf{x}|T_{\mathfrak{A}} + T_{\mathfrak{A}}|\mathbf{x}| \geq 0$$

on $C_0^\infty(\mathbb{R}^d)$.

Proof. By the diamagnetic inequality (Theorem 18)

$$(9) \quad (\eta, |\mathbf{p}||\phi|) \leq \Re(\eta, \text{sgn}(\phi)|\mathbf{p} + \mathfrak{A}|\phi)$$

we see that $|\mathbf{x}||\mathbf{p}| + |\mathbf{p}||\mathbf{x}| \geq 0$ implies $|\mathbf{x}||\mathbf{p} + \mathfrak{A}| + |\mathbf{p} + \mathfrak{A}||\mathbf{x}| \geq 0$. In other words, it suffices to prove positivity without the background magnetic field. Moreover: it suffices to consider $\phi \geq 0$.

Next we recall the following representation of $|\mathbf{p}|$ (Lieb and Yau [6]) in position space

$$(10) \quad (\psi, |\mathbf{p}|\psi) = \alpha_d \int_{\mathbb{R}^d} d\mathbf{x} \int_{\mathbb{R}^d} d\mathbf{y} \frac{(\overline{\psi(\mathbf{x})} - \overline{\psi(\mathbf{y})})(\psi(\mathbf{x}) - \psi(\mathbf{y}))}{|\mathbf{x} - \mathbf{y}|^{d+1}}$$

with $\alpha_d = \Gamma(\frac{d+1}{2})/(2\pi^{\frac{d+1}{2}})$. By polarization of (10) Inequality (8) is then equivalent to

$$(11) \quad 0 \leq t := \Re \int_{\mathbb{R}^d} d\mathbf{x} \int_{\mathbb{R}^d} d\mathbf{y} \frac{(\overline{\psi(\mathbf{x})} - \overline{\psi(\mathbf{y})})(|\mathbf{x}|\psi(\mathbf{x}) - |\mathbf{y}|\psi(\mathbf{y}))}{|\mathbf{x} - \mathbf{y}|^{d+1}}$$

where we restrict to non-negative ψ because of the above remark. Now, setting $\psi = g/|\cdot|^{d/2}$ and regularizing to avoid the singularity at $\mathbf{x} = \mathbf{y}$ we get

$$(12) \quad \begin{aligned} t &= \lim_{\epsilon \rightarrow 0} \Re \int_{\mathbb{R}^d} d\mathbf{x} \int_{\mathbb{R}^d} d\mathbf{y} \frac{\frac{|\mathbf{x}|g(\mathbf{x})^2}{|\mathbf{x}|^d} + \frac{|\mathbf{y}|g(\mathbf{y})^2}{|\mathbf{y}|^d} - g(\mathbf{x})g(\mathbf{y})\frac{|\mathbf{y}|+|\mathbf{x}|}{|\mathbf{x}|^{d/2}|\mathbf{y}|^{d/2}}}{|\mathbf{x} - \mathbf{y}|^{d+1} + 2^{\frac{d+1}{2}}\epsilon(|\mathbf{x}|^{d+1} + |\mathbf{y}|^{d+1})} \\ &= \lim_{\epsilon \rightarrow 0} \int_{\mathbb{R}^d} d\mathbf{x} \frac{g(\mathbf{x})^2}{|\mathbf{x}|^d} \int_{\mathbb{R}^d} d\mathbf{y} \frac{2 - |\mathbf{y}|^{1-d/2} - |\mathbf{y}|^{-d/2}}{|\mathbf{e} - \mathbf{y}|^{d+1} + 2^{\frac{d+1}{2}}\epsilon(1 + |\mathbf{y}|^{d+1})} \\ &\quad + \frac{1}{2} \int_{\mathbb{R}^d} d\mathbf{x} \int_{\mathbb{R}^d} d\mathbf{y} \frac{(|\mathbf{x}| + |\mathbf{y}|)(g(\mathbf{x}) - g(\mathbf{y}))^2}{|\mathbf{x}|^{d/2}|\mathbf{x} - \mathbf{y}|^{d+1}|\mathbf{y}|^{d/2}} \\ &\geq \int_{\mathbb{R}^d} d\mathbf{x} \frac{g(\mathbf{x})^2}{|\mathbf{x}|^d} \int_0^\infty \frac{dr r^d}{r} (2 - r^{1-d/2} - r^{-d/2})(2r)^{-\frac{d+1}{2}} \\ &\quad \cdot \int_{\mathbb{S}^{d-1}} \frac{d\omega}{\left(\frac{r+r^{-1}}{2} - \omega\mathbf{e}\right)^{\frac{d+1}{2}} + \epsilon\left(\frac{1}{r}^{\frac{d+1}{2}} + r^{\frac{d+1}{2}}\right)} \\ &\geq 2^{-\frac{d+1}{2}} \int_{\mathbb{R}^d} d\mathbf{x} \frac{g(\mathbf{x})^2}{|\mathbf{x}|^d} \int_0^\infty \frac{dr}{r} (2r^{\frac{d-1}{2}} - r^{1/2} - r^{-1/2}) \\ &\quad \cdot \int_{\mathbb{S}^{d-1}} \frac{d\omega}{\left(\frac{r+r^{-1}}{2} - \omega\mathbf{e}\right)^{\frac{d+1}{2}} + \epsilon\left(\frac{1}{r}^{\frac{d+1}{2}} + r^{\frac{d+1}{2}}\right)} \\ &\geq 2^{-\frac{d+1}{2}} \int_{\mathbb{R}^d} d\mathbf{x} \frac{g(\mathbf{x})^2}{|\mathbf{x}|^d} \int_0^\infty \frac{dr}{r} \underbrace{\left[r^{\frac{d-1}{2}} + r^{-\frac{d-1}{2}} - (r^{\frac{1}{2}} + r^{-\frac{1}{2}})\right]}_{\geq 0} \\ &\quad \cdot \int_{\mathbb{S}^{d-1}} \frac{d\omega}{\left(\frac{r+r^{-1}}{2} - \omega\mathbf{e}\right)^{\frac{d+1}{2}} + \epsilon\left(\frac{1}{r}^{\frac{d+1}{2}} + r^{\frac{d+1}{2}}\right)} \geq 0 \end{aligned}$$

where \mathbf{e} is any unit vector in \mathbb{R}^3 . The positivity of the bracket follows from the fact that the function $f(\alpha) := r^\alpha + r^{-\alpha}$ is strictly monotone increasing for positive r . \square

We remark that the above proof also shows that $d = 2$ is borderline for positivity. In fact,

$$|\mathbf{x}||\mathbf{p}| + |\mathbf{p}||\mathbf{x}| \geq 2\alpha_d\gamma_d$$

where

$$(13) \quad \gamma_d = 2^{-\frac{d-1}{2}} \int_0^1 \frac{dr}{r} [r^{\frac{d-1}{2}} + r^{-\frac{d-1}{2}} - (r^{\frac{1}{2}} + r^{-\frac{1}{2}})] \int_{\mathbb{S}^{d-1}} \frac{d\omega}{\left(\frac{r+r^{-1}}{2} - \omega \mathbf{e}\right)^{\frac{d+1}{2}}}$$

which changes sign at $d = 2$ whereas $|\mathbf{x}||\mathbf{p}| + |\mathbf{p}||\mathbf{x}| \geq 1$ for $d = 3$.

3. APPLICATION TO $2d$ QUANTUM DOTS

In this section we consider a $2d$ quantum dot given by the Hamiltonian

$$(14) \quad C_{A,\varphi,N} := \sum_{n=1}^N [|\mathbf{p} + \mathfrak{A}|_n + e\boldsymbol{\sigma}_n \cdot \mathbf{A}(\mathbf{x}_n) - e\varphi(\mathbf{x}_n)] + \sum_{1 \leq m < n \leq N} \frac{e^2}{|\mathbf{x}_m - \mathbf{x}_n|},$$

a simplified model of (3), self-adjointly realized in $\mathfrak{H}_N := \bigwedge_{n=1}^N L^2(\mathbb{R}^2 : \mathbb{C}^2)$. Here \mathfrak{A} is the background magnetic field (4) and \mathbf{A} is the magnetic field defining the dot. Furthermore, we allow for an attractive essentially spherically symmetric attractive potential. We have

Theorem 2. *Assume $\mathfrak{A} \in L^2_{\text{loc}}(\mathbb{R}^2 : \mathbb{R}^2)$ and $|\mathbf{A}(\mathbf{x})| \leq e\delta/|\mathbf{x}|$, $\varphi(\mathbf{x}) \leq eZ/|\mathbf{x}|$, $Z \in [0, \kappa_k]$. Assume that $C_{A,\varphi,N}$ has a ground state with ground state energy E_N below the saturation threshold, i.e., $E_N < E_{N-1}$. Then*

$$N < 2(\delta + Z) + 1.$$

Note that our bound – in the absence of an electric potential – grows linearly in the missing magnetic flux μ which, in the case of (5), equals $\mu = e\delta = R^2 B e / 2$.

Equipped with Inequality (8) the proof follows now the lines of Lieb's original proof.

Proof. Assume that there is ground state ψ of $C_{A,\varphi,N}$, i.e.,

$$(15) \quad C_{A,\varphi,N}\psi = E_N\psi$$

with E_N . We begin by singling out the first coordinate and multiplying (15) by $|\mathbf{x}_1|\psi$ and obtain using (8) and a standard density argument (approximating ψ by C_0^∞ functions)

$$(16) \quad \begin{aligned} & e^2(|\mathbf{x}_1|\psi, [-(\delta + Z)/|\mathbf{x}_1| + \sum_{n \neq 1} \frac{1}{|\mathbf{x}_1 - \mathbf{x}_n|}]\psi) \\ & < (|\mathbf{x}_1|\psi, [C_{A,\varphi,1} - e^2 \sum_{n \neq 1} |\mathbf{x}_1 - \mathbf{x}_n|^{-1}]\psi + 1 \otimes (C_{A,\varphi,N-1} - E_{N-1})\psi) \\ & = (E_N - E_{N-1})(|\mathbf{x}_1|\psi, \psi) < 0. \end{aligned}$$

Repeating the same argument for all the other coordinates $\mathbf{x}_2, \dots, \mathbf{x}_n$ and summing the result, gives

$$(17) \quad -(\delta + Z)N + \frac{1}{2} \sum_{\substack{m,n=1 \\ m \neq n}}^N \frac{|\mathbf{x}_m| + |\mathbf{x}_n|}{|\mathbf{x}_m - \mathbf{x}_n|} < 0.$$

Thus the triangle inequality implies

$$-(\delta + Z)N < \frac{N^2 - N}{2}$$

which is the claimed result. \square

APPENDIX A. AUXILIARY RESULTS

Theorem 3. For $\phi, \eta \in H^1(\mathbb{R}^d)$, $\eta \geq 0$, $m \in \mathbb{R}_+$, $T_m(\mathbf{p}) = \sqrt{\mathbf{p}^2 + m^2} - m$, $\mathfrak{A} \in L^2_{\text{loc}}(\mathbb{R}^3)$ and $\mathbf{p} = -i\nabla$ we have

$$(18) \quad (\eta, T_m(\mathbf{p})|\phi|) \leq \Re(\eta, \text{sgn}(\phi)T_m(\mathbf{p} + \mathfrak{A})\phi).$$

This is Kato's inequality for the Chandrasekhar operator (Simon [13], Könenberg et al [4]).

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